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A modification of usual C–V measurement to more precisely characterize the band offsets in a-Si:H/c-Si heterojunctions

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ABSTRACT

Due to a strong inversion layer at the a-Si:H/c-Si interface, there are errors in the determination of the band offsets by usual capacitance–voltage (C–V) measurements. An improved C–V measurement was presented to correct the errors by a modification to the apparent diffusion potential V_{int}. In this paper, the improved C–V measurement is used to characterize the band offsets in a-Si:H/c-Si heterojunctions with a good precision. The modified apparent diffusion potential is determined from V_{int} and the minority carrier density at the c-Si interface deduced from the coplanar conductance measurements. The value of $\Delta E_C = 0.17 \pm 0.04$ eV between a-Si:H and c-Si is found by the improved C–V measurement with a precise determination of the band offsets.

Introduction

The band offsets are very important parameters which play the key role in any heterojunction device. Particularly for amorphous hydrogenated silicon/crystalline silicon (a-Si:H/c-Si) heterojunction solar cells, the parameters determine the equilibrium band diagram, the carrier transport mechanism and the passivation efficiency at front and rear interfaces [1–3]. Consequently, a variety of techniques have been developed to investigate the band offsets [1,4–7]. Among such techniques, the capacitance–voltage (C–V) measurements are proposed as one of the easiest and most used technique to get insights into the band offsets. The approach has been used to determine the band offsets in a-Si:H/c-Si heterojunctions by several authors [8]. As is clear from the equilibrium band diagram of a-Si:H/c-Si heterojunctions shown in Fig. 1, the conduction band offset in the heterojunction is obtained by

$$\Delta E_C = \delta_1 + \delta_2 + qV_D - E_{g1}, \qquad (1)$$

where V_D is the diffusion potential, δ_1 and δ_2 are energy differences between the Fermi level and the nearest band edge of c-Si and a-Si:H, and E_{g1} and E_{g2} are the band gaps of c-Si and a-Si:H. It is widely assumed that V_D is estimated from the intercept of the linear extrapolation of $1/C^2$ with the voltage axis, V_{int}.

Although the C–V method is a straightforward tool for the determination of the band offsets, there may be errors in the determination of the band offsets of a-Si:H/c-Si heterojunctions from the usual C–V method due to several sources of errors [6–10]. It is reported that the presence of a strong inversion layer in c-Si or non-negligible interface states affects the apparent diffusion potential V_{int} and then results in errors in the determination of the band offsets when taking V_{int} as V_D [11–13]. The passivation of c-Si surfaces by an intrinsic a-Si:H ((i) a-Si:H) layer leads to very low effective surface recombination velocities so that errors due to interface states can be eliminated [14]. Although, due to the inversion layer at the c-Si interface, taking V_{int} as the experimental determination of the diffusion potential may obviously result in errors in the determination of the conduction band offset ΔE_C, especially at high values of ΔE_C [15]. Recently, by taking account of the charge effect of the strong inversion layer, the theoretical capacitance of a-Si:H/c-Si heterojunctions in high frequency including the effect of a strong inversion layer was developed to modify the apparent diffusion potential. The modified apparent diffusion potential almost agrees well with the theoretical value for various conduction band offsets. In this paper, the improved C–V measurement is used to characterize the band offsets in (n^+) a-Si:H/(p) c-Si heterojunctions with good precision.

Experiments

a-Si:H/c-Si heterojunctions were fabricated by PECVD deposition of n^+-type a-Si:H layer onto p-type crystalline Si substrate (FZ, 1–5 Ω cm, (1 1 1), 300 μm) with Al back surface field and glass at a substrate temperature of 200 °C. The thickness of the

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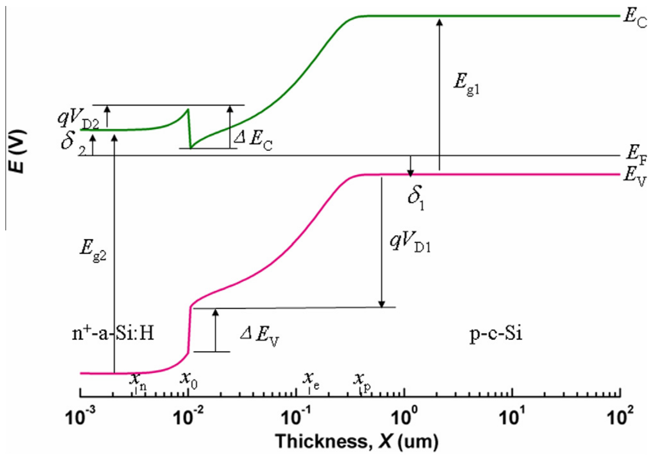

Fig. 1. Energy band diagram of an abrupt (n+) a-Si:H/(p) c-Si heterojunction at equilibrium.

(n+) a-Si:H emitter was kept at about 20 nm. Prior to the deposition, the c-Si surface was prepared by removing the native oxide using a wet chemical etching procedure (HF diluted at 5% in water). A series of samples were fitted with top parallel coplanar aluminum electrodes. The samples were analyzed using dark current measurements in a wide range of temperatures [150–370 K] in a cryostat chamber pumped down to 10^{-5} mbar. For a second series of samples, a TCO layer (80 nm) was deposited by RF-magnetron sputtering. The structures were completed by screen printing of Ag grids. The capacitance measurements of the samples as a function of bias, C–V, were performed in a vacuum cryostat at 300 K using an impedance meter at the frequency of 100 kHz.

Results and discussion

By taking account of the charge effect of the strong inversion layer, the theoretical capacitance of (n+) a-Si:H/(p) c-Si heterojunctions in high frequency including the effect of a strong inversion layer is developed by [15]

$$C^{-2} = \frac{2}{q\varepsilon_s N_{A1}}[V_D - V - \beta n_1(x_0)/n_{D2}] \tag{2}$$

with $\beta = kT/q$, where $n_1(x_0)$ is the minority carrier density at the c-Si interface ($x = x_0$), ε_s is the dielectric constants of silicon materials, N_{A1} is the impurity concentration of c-Si, and n_{D2} is the majority carrier density in a-Si:H. The apparent diffusion voltage, V_{int}, obtained by extrapolating the slope of $1/C^2$ at low reverse bias and forward bias to zero, can be determined from Eq. (2) and is given by [15]

$$V_{\text{int}} = V_D - \beta n_1(x_0)/n_{D2} \tag{3}$$

There is a difference $\beta\frac{n_1(x_0)}{n_{D2}}$ between the apparent diffusion potential V_{int} and the theoretical value of V_D. To illustrate the errors in the determination of the band offsets, numerical simulations of V_{int} and V_D for various values of ΔE_C are performed using a numerical PC program, AFORS–HET [16]. The density of gap states (DOS) adopted for a-Si:H is composed of two exponential Urbach tail states distributions and two Gaussian midgap states distributions [17]. The material parameters used in the numerical simulations for the c-Si and a-Si:H layers are given in Table 1, where G_{AO} and G_{DO} are the prefactors, E_A and E_D are the tail characteristic energies, G_{Ga} and G_{Gd} are the prefactors, E_{pka} and E_{pkd} are the peak energies, and δ_d and δ_a are the standard deviations. No interface state is introduced. The calculated values of V_D and V_{int} are plotted versus ΔE_C in Fig. 2. Due to a strong inversion layer, taking V_{int} as V_D results in obvious errors in the determination of the band offsets above ΔE_C = 0.05 eV from the usual C–V method, especially at high values of ΔE_C. Furthermore, errors increase with an increasing ΔE_C. An improved C–V measurement was presented to correct the errors by a modification to V_{int}. Deduced from Eq. (3), the diffusion potential, which is marked as the modified diffusion potential, is obtained as

$$V^*_{\text{int}} = V_{\text{int}} + \beta n_1(x_0)/n_{D2} \tag{4}$$

The modified apparent diffusion potential V^*_{int} calculated from the parameters n_{D2} and $n_1(x_0)$ also is shown in Fig. 2. As seen in Fig. 2, V^*_{int} almost agrees well with V_D. The band offsets can be determined more precisely from V_{int} as well as $n_1(x_0)$ than usual.

The modified apparent diffusion potential V^*_{int} can be calculated from the parameters n_{D2} and $n_1(x_0)$. From the equilibrium band diagram of (n+) a-Si:H/(p) c-Si heterojunctions shown in Fig. 1, the minority carrier density at the c-Si interface, $n_1(x_0)$, can be deduced from the energy difference between the Fermi level and the nearest band edge at the c-Si interface, which is the activation energy of the conductance at the interface, E_a, which can be determined from static coplanar conductance measurements [18,19].

The experimental plot of $1/C^2$ versus applied bias at the frequency of 100 kHz is shown in Fig. 3. The curves have a well-defined linear behavior at reverse bias and small forward bias. In this case, the impurity concentration of c-Si wafers, N_{A1}, may be obtained from the slope of the plots. We find the value of

Table 1
Main parameters of a-Si:H/c-Si heterojunction layers used in simulations.

Parameter	(n) a-Si:H	c-Si
Band gap (eV)	1.8	1.12
Thickness (nm)	10	3×10^5
N_{A1} and n_{D2} (cm^{-3})	1×10^{19}	10^{16}
Electron affinity (eV)	3.65–4.05	4.05
G_{AO} and G_{DO} (cm^{-3})	10^{21}	10^{14}
E_D (eV)	0.05	0.01
E_A (eV)	0.036	0.01
G_{Ga} and G_{Gd} (cm^{-3})	2.4×10^{19}	10^{12} (constant)
E_{pkd} (eV)	0.96	–
E_{pka} (eV)	0.56	–
δ_d and δ_a (eV)	0.15	–

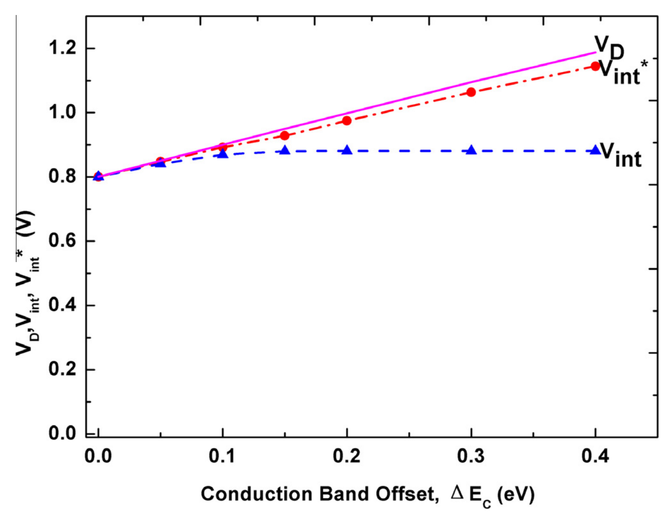

Fig. 2. Calculated plot of the diffusion potential, V_D, (solid lines), the intercept of the linear part of simulated $1/C^2$ curves with bias axis, V_{int}, (dashed lines with symbols), and the modified intercept, V^*_{int}, (dash dot lines with symbols), versus conduction band offset, ΔE_C.

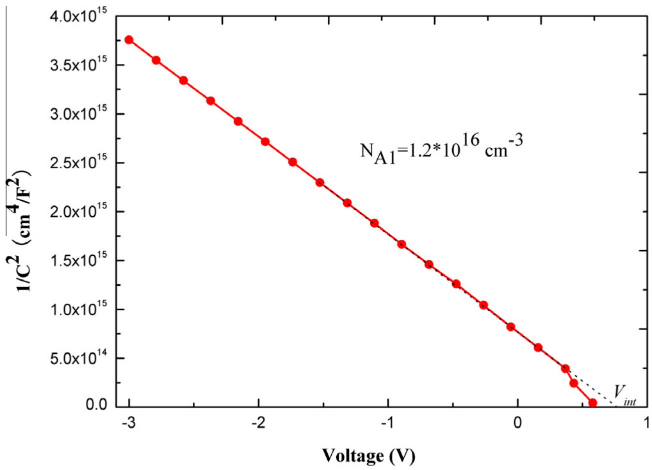

Fig. 3. Experimental $1/C^2$ curves versus applied bias obtained at 100 kHz.

$1.2 \pm 0.1 \times 10^{16}\ \text{cm}^{-3}$. This value is in agreement with the nominal resistivity of the silicon wafers (1–5 Ω cm). As can be seen from Fig. 3, the intercept of the plot with the bias axis, V_{int}, is equal to 0.82 V.

The dark conductance is given by

$$\sigma = Il/LUd \tag{5}$$

where I is the current, l is the distance between two coplanar electrodes, L is the length of electrodes and d is the width between electrodes. Also, the dark conductance can be expressed as

$$\sigma = \sigma_0 \exp(-E_a/kT) \tag{6}$$

Arrhenius plots of the conductance for the two types of samples, which is deduced from dark current measurements, are shown in Fig. 4. The conductance of the a-Si:H/c-Si heterojunction samples is much higher than that of the a-Si:H/glass ones. Also, the values of the activation energy of the conductance are very different between the two types of samples. While typical values around 0.18 ± 0.02 eV for n-type a-Si:H are found for the a-Si:H/glass samples, much lower values around 0.019 ± 0.002 eV are obtained for the a-Si:H/c-Si heterojunction samples, which demonstrates the existence of the strong inversion layer at the heterojunction

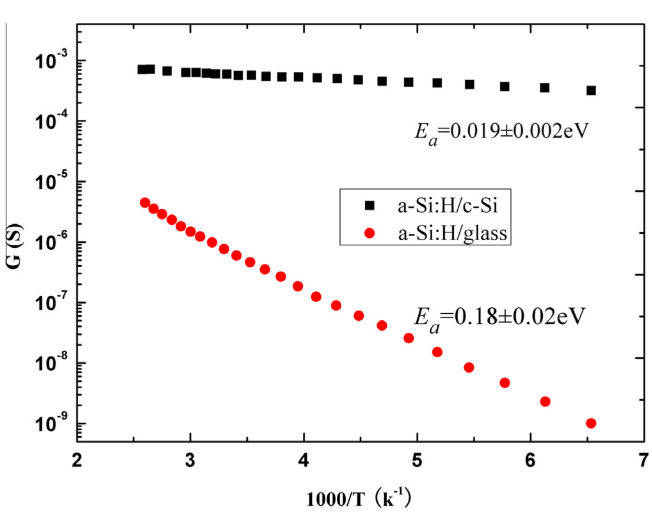

Fig. 4. Temperature dependence of the conductance for a-Si:H/c-Si interface and a-Si:H/glass layers.

interface [20–22]. Determined from the improved C–V measurements (Eqs. (1) and (3)), the value of $\Delta E_C = 0.17 \pm 0.04$ eV is found for the conduction band offset between a-Si:H and c-Si. As seen in Fig. 2, there are errors in the determination of the band offsets for a-Si:H/c-Si heterojunctions from the improved C–V methods. As is reported [7,8], it demonstrates that the band offset is mainly concentrated in the valence band.

Conclusions

The improved C–V measurement was presented to precisely determine the band offsets between a-Si:H and c-Si by a modification to the apparent diffusion potential V_{int}. Then the improved C–V measurement is applied to characterize the band offsets from apparent diffusion potential measurements and static coplanar conductance measurements. Determined from the apparent diffusion potential V_{int} and the minority carrier density at the c-Si interface deduced from the coplanar conductance measurements, the value $\Delta E_C = 0.17 \pm 0.04$ V between a-Si:H and c-Si is found by the improved C–V measurement.

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